2,2',5,5'-tetrachloro-4-methyl-diphenylmethane

Other names: 2,2',5,5'-tetrachlorobenzyl 4-toluene
Inchi: InChI=1S/C14H10Cl4/c1-8-4-14(18)10(7-13(8)17)5-9-6-11(15)2-3-12(9)16/h2-4,6-7H,5H2
InchiKey: FLNHUBDFYWZFMU-UHFFFAOYSA-N
Formula: C14H10Cl4
SMILES: Cc1cc(Cl)c(Cc2cc(Cl)ccc2Cl)cc1Cl
Mol. weight [g/mol]: 320.04

Physical Properties

Property code	Value	Unit	Source
gf	195.95	kJ/mol	Joback Method
hf	20.46	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-8.03		Aqueous Solubility Prediction Method
logp	6.199		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2135.20		NIST Webbook
rinpol	2145.20		NIST Webbook
tb	747.70	K	Joback Method
tc	1002.50	K	Joback Method
tf	482.66	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.32	J/mol×K	747.70	Joback Method
cpg	477.97	J/mol×K	790.17	Joback Method
cpg	488.65	J/mol×K	832.63	Joback Method
cpg	498.43	J/mol×K	875.10	Joback Method
cpg	507.35	J/mol×K	917.56	Joback Method
cpg	515.47	J/mol×K	960.03	Joback Method

cpg	522.84	J/mol×K	1002.50	Joback Method
dvisc	0.0006543	Pa×s	482.66	Joback Method
dvisc	0.0004524	Pa×s	526.83	Joback Method
dvisc	0.0003312	Pa×s	571.01	Joback Method
dvisc	0.0002535	Pa×s	615.18	Joback Method
dvisc	0.0002012	Pa×s	659.35	Joback Method
dvisc	0.0001643	Pa×s	703.53	Joback Method
dvisc	0.0001375	Pa×s	747.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R181190&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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